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DIFFERENTIAL ENTROPY PER PARTICLE IN WEYL SEMIMETALS

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Abstract

In this work we theoretically investigate the behavior of enthropy per particle, $\partial S/\partial n$ in Weyl semimetals. The impact of magnetic field is also discovered. It is shown that entropy in magnetic field undergo oscillations due to presence of Landau levels in the energy spectrum. Entropy oscillations in Weyl semimetals are compared with same for 2D Dirac materials, for which the analytic expression is obtained for the first time. The limit of zero magnetic field is also discovered; the analytic expression for entropy in this case is also got.

Keywords: weyl semimetals, entropy, dirac materials

Introduction

Dirac materials and, partially, Weyl semimetals are facing increasing interest last years [1]. Although it is not clear yet that any of existing compounds can be finally recognized as true Weyl semimetal, various possible practical implementations of Weyl SM were already proposed [2]. At the same time V. Yu. Tsaran et al [3] shown that differential entropy per particle $\partial S/\partial n$ in 2D Dirac systems can represent important features of the Fermi surface. The experimental method of measuring this value was also proposed [4].
In this paper we discover the enropy per particle for Weyl semimetals, and its behaviour in magnetic field.

1. Energy spectrum and density of states

A three-dimensional Dirac semimetal is a material in which the conduction and valence bands touch at isolated points, called Dirac points, within the Brillouin zone (BZ). Around these points the dispersion is linear and the low energy theory at two Dirac points K and K' of oppose chirality ξ is described by the Hamiltonian,

$$H = \begin{pmatrix} \hbar v_F \sigma \mathbf{k} & 0 \\ 0 & -\hbar v_F \sigma \mathbf{k} \end{pmatrix}, \tag{1}$$

where v_F is Fermi velocity, σ – Pauli matrices, k is momentum. Let us consider a magnetic field along z axis, $\mathbf{B} = \mathbf{B}\hat{z}$, and use the gauge $A_y = A_z = 0$ and $A_x = -B_y$. The spectrum at $K(\xi = 1)$ and $K'(\xi = -1)$ points is presented on Fig. 1, and is given by the expressions

$$E_{0\xi} = -\xi \hbar v_F k_z, \tag{2}$$

$$E_{n\xi\lambda} = \sqrt{(\hbar v_F k_z)^2 + \Delta_n^2} \tag{3}$$

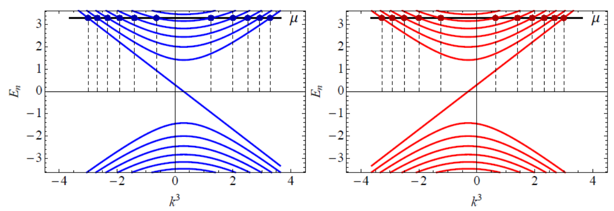

Fig. 1. Energy spectrum of Weyl semimetal in magnetic field. Left pannel:K point, right pannel: K' point

Density of states is given by [5]:

$$D(\varepsilon) = \frac{1}{2\pi^2 \hbar v_F l^2} \left[1 + 2\sum_{n=1}^{\infty} \frac{|\varepsilon|}{\sqrt{\varepsilon^2 - \Delta_n^2}} \theta(\varepsilon^2 - \Delta_n^2) \right], \tag{4}$$

where Δ_n – the breadth of n-th Landau level, l – the magnetic length.

The limit of zero magnetic field is obtained by keeping the level breadth Δ constant, while $B \to 0, n \to 0$:

$$\lim_{B \to 0} D(\varepsilon) = \frac{\varepsilon^2}{\pi^2 (\hbar v_F)^3} \tag{5}$$

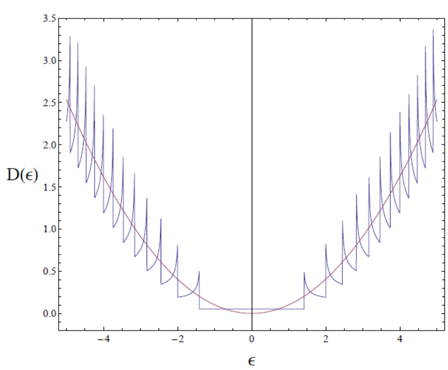

Fig. 2. Density of states

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2. Entropy per particle in magnetic field

From thermodynamics we can express entropy per particle as

$$s = \left(\frac{\partial S}{\partial n}\right)_T = -\left(\frac{\partial \mu}{\partial T}\right)_n = \left(\frac{\partial n}{\partial T}\right)_\mu \left(\frac{\partial n}{\partial \mu}\right)_T^{-1} \qquad (6)$$

Using the fact that

$$n(\mu, T) = \int_{-\infty}^{\infty} D(\varepsilon) f_{FD}(\mu, T), \qquad (7)$$

where f_{FD} is Fermi-Dirac distribution, we get a final expression for s:

$$s(\mu, T) = \frac{1}{T} \frac{\int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)(\varepsilon - \mu)\cosh^{-2}\left(\frac{\varepsilon-\mu}{2T}\right)}{\int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)\cosh^{-2}\left(\frac{\varepsilon-\mu}{2T}\right)} \qquad (8)$$

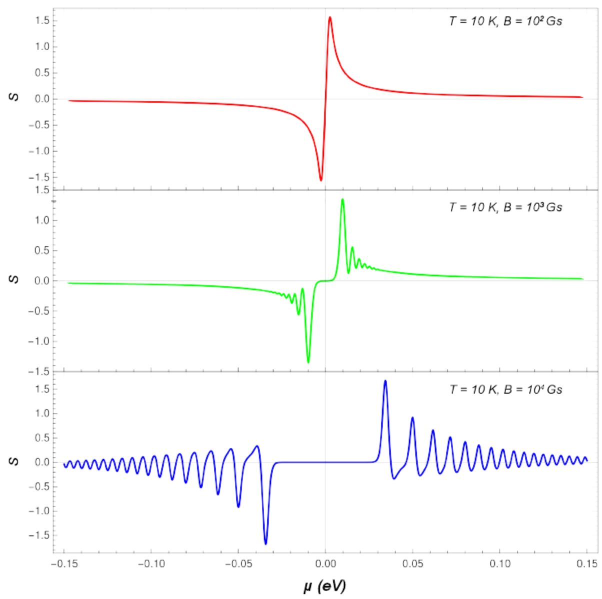


Fig. 3. Entropy per particle vs chemical potential at temperature of 10K for three values of magnetic field (up to down): 10^2Gs, 10^3Gs, 10^4Gs

Limit $T \to 0$ gives:

$$\frac{\partial n}{\partial T} \to \frac{\pi^2 T}{3} \frac{dD(\mu)}{d\mu} \qquad (9)$$

$$\frac{\partial n}{\partial \mu} \to D(\mu) \qquad (10)$$

2.1. Comparison with 2D case

According to the work [6], density of states for planar Dirac system in magnetic field in absence of gap is:

$$D_{2D}(\varepsilon) = \frac{1}{2\pi\hbar v_F l} \frac{d}{d\varepsilon}\left(1 + 2\sum_{n=1}^{\infty} \theta(e^2 - \Delta_n^2)\right) \qquad (11)$$

Implementing formula (8), we get:

$$s_{2D} = \frac{\sum_n \Delta_n \left(\cosh^{-2}(\frac{\Delta_n-\mu}{2T}) - \cosh^{-2}(\frac{\Delta_n+\mu}{2T})\right)}{T\sum_n \left(\cosh^{-2}(\frac{\Delta_n-\mu}{2T}) + \cosh^{-2}(\frac{\Delta_n+\mu}{2T})\right)} - \frac{\mu}{T} \qquad (12)$$

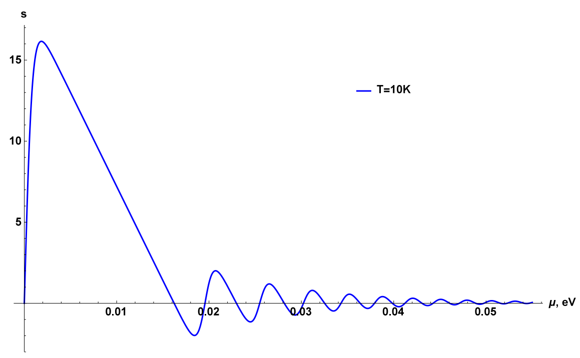


Fig. 4. Entropy vs chemical potential for 2D Dirac system at the temperature of 10K and field $2 \cdot 10^3$Gs.

We can see that peaks of entropy differ from 2D to 3D case. Those peaks for 2D systems seem to infinitely grow due to the abscence of scattering in this model.

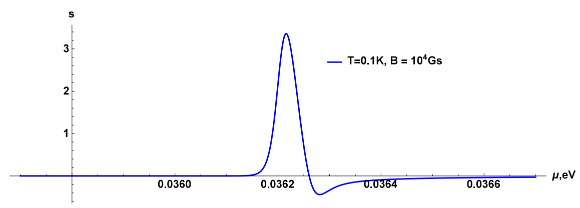


Fig. 5. First peak of $s(\mu)$ at $T = 0.1K, B = 10^4 Gs$.

The shape of peaks is the same for positive and negative ones. But in 3D, the negative peaks for positive values of μ, and positive peaks for negative μ have another shape. Moreover, they not tend to grow infinitely, as it is shown for first peak in positive range of μ on Fig. 5. This behaviour prenends to be an unique feature of Weyl SM.

3. Entropy without field

Using density of states for zero field limit, equation. 5 and formula. 8, we get the entropy in abscence of magnetic field:

$$s_0(\mu, T) = \frac{2\mu T}{T^2 + \frac{3}{\pi^2}\mu} \qquad (13)$$

The function $s_0(\mu, T)$ takes its maximum value $s_{0max} = \frac{\pi}{\sqrt{3}}$ at the point $\mu_{max} = \pi T/\sqrt{3}$. It is remarkable that s_{0max} does not depend on temperature.

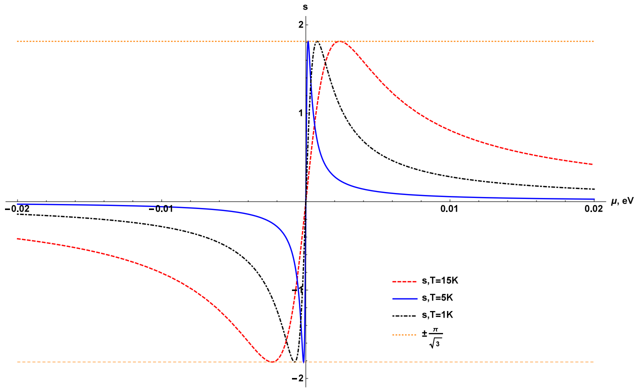


Fig. 6. Entropy per particle as function of chemical potential. Limit of zero magnetic field

One also can get assymptotic behaviour of s_0 :

$$s_0 = \begin{cases} \frac{2\pi^2}{3}\frac{T}{\mu}, & \frac{T}{\mu} \to 0 \\ \frac{2\mu}{T} & \frac{\mu}{T} \to 0 \end{cases} \quad (14)$$

4. Surface effects

One of the key features of Weyl semimetals is presence of Fermi arcs at their surface states [7]. It was widely studied in the work [8]. From there we take density of states on the surface:

$$D_{surf}(\varepsilon) = \frac{|eB|(L + k_0\hbar c/|eB|)}{2\pi^4\hbar cL}\cdot$$
$$\cdot\mathrm{Im}\left[\Psi\left(n_{min} + \frac{(\varepsilon + i\Gamma)(L + k_0\hbar c/|eB|)}{\pi\hbar v_F}\right) + \right. \quad (15)$$
$$\left. + \ \Psi\left(n_{min} - \frac{(\varepsilon - i\Gamma)(L + k_0\hbar c/|eB|)}{\pi\hbar v_F}\right)\right],$$

where Ψ is digamma function, $n_{min} = \left[\frac{\mu L}{\pi v_F} + 1\right]$ (the brackets [ ] mean integer part); k_0 is the arc length in momentum space, L is sample width, Γ is scattering parameter.

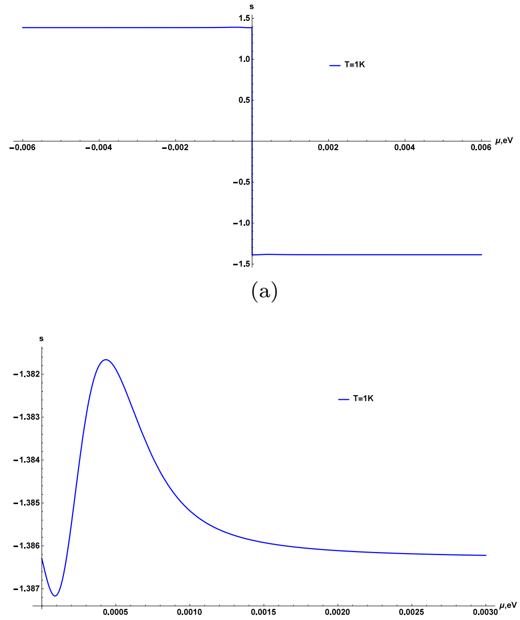
Using this DOS and equation 8, we can plot the entropy per particle on surface of Weyl semimetal. Parameters for DOS here is the same as in the study [8]

Here we can see that with chosen parameters, enthropy per particle behaves nearly as constant value on the surface, but also exhibit minimum and maximum value.

While measuring s in experiment, both surface and bulk entropy contributions should be taken into account.

Conclusions

The dependencies of entropy per particle on chemical potetnial were analyzed for Weyl semimetal. Finite maxima were revealed, in contrast to 2D dirac materials. Assymptotic behaviour of was studied: analytical expressions of $T \to 0$ and $B \to 0$ were obtained. Entropy per particle of the surface states was also plotted and discussed. A pair of maximum and minimum were detected for this case. All of this may advance futher research by revealing characteristic features of Weyl semimetals, which can be measured, and so it may help detect whether a some material is Weyl semimetal or not.



(a)

(b)

Fig. 7. Entropy per particle on the surface of Weyl SM at the temperature of 1K as function of chemical potential. (a): overall plot; (b): vincinity of maximum

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